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RE-ENTRANCE AND COEXISTENCE OF SUPERCONDUCTIVITY WITH SPIN DENSITY WAVE SYSTEMS

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Abstract : The coexistence of spin density wave (SDW) state and superconductivity (SC) is studied within the mean field theory. The SDW instability is driven by the existence of nested pieces of Fermi surface(FS) in presence of intermediate Coulomb repulsion strength whereas the superconductivity is mediated by some boson exchange. Furthermore, the SDW order exist only in those parts of the FS where it nests whereas the superconducting correlation exists all over the FS. Under such a situation, when the interaction strengths for the SC and SDW instabilities are comparable to each other, we find strong competing and re-entrant behaviour ; presence of one inhibiting the other. Such strong competition between magnetism and superconductivity is seen in recently discovered borocarbides and could be applicable to wide classes of superconductors and cuprates.

Keywords : Nesting of Fermi surface, Re-entrant magnetism, spin density wave, Borocarbides.

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The coexistence of magnetism and superconductivity has intrigued both exprimentalists and theoreticians for a long time. Specially, whether superconductivity and magnetic order can occur within the same volume element in a substance and, if so, under what conditions, has been of immense interest. It is well known that the superconductivity (SC) and spin density wave (SDW) co-exist in a large classes of systems e.g., organic layered superconductors [1], the Bechgaard salts $(TMTSF)X$, with $X = PF_6$, AsF_6, ClO_4 etc. [2], heavy fermion systems [3], high temperature superconductors [4] and recently discovered borocarbides [5].

In case of the organic superconductors belonging to the family $(TMTSF)_2X$ ($TMTSF \equiv$ tetramethyltetraselena fulvalene and $X = PF_6$, AsF_6 etc.) show coexistence of superconductivity and spin density wave type antiferromagnetism (SDW) at low temperature in moderate pressures ($\sim$ 7 Kbar) [6]. Many compounds ($X = PF_6$, AsF_6, SbF_6 etc.) exhibit metal - insulator transition at 12 - 17 K under ambient pressure which is caused by spin density wave (SDW) transition. This transition is suppressed by moderate pressures which results in superconductivity. However, the nature of this coexistence is very much different from what would encounter in case of ternary compounds. In organic superconductors, there is only one conduction band and the antiferromagnetic ordering destroys the Fermi surface (FS) due to its $2k_F$ periodicity which results in an insulating phase. In high-T_c cuprates also due to the low dimensionality aspects there exists similar periodicity known as nesting of the FS [7], and leads to FS instability by forming the SDW state. On the other hand, in intermetallic compounds the magnetism is due to localized f electrons and superconductivity arises due to the conduction electrons. These organic superconductors in turn, are essentially quasi one dimensional compounds with weak interaction between the adjacent chains. In the present paper we shall discuss about the possible co-existence of SC and SDW, where the SDW exists only in particular direction of the FS due to its particular topology (nesting) and in the other directions the cooper pairing leads to superconductivity.

The SDW transition occurs when the spatial spin density modulation is due to delocalization or initinerant electrons rather than the localized one. In the normal state the density $\rho_\uparrow(\vec{r})$ of electron spins polarized upward with respect to any quantization axis is completely cancelled by $\rho_\downarrow$ of downward polarized spins. In the SDW state, however, the difference $\sigma(\vec{r}) = \rho_\uparrow(\vec{r}) - \rho_\downarrow(\vec{r})$ is finite. and modulate in space as a fuction of the position vector $\vec{r}$ in the SDW state. Such tendency of forming SDW ground state takes place when a system possesses nested pieces of FS together with intermidiate coulomb correlation. In the case of the SDW transition it is the wave vector dependent static magnetic susceptibility which develops a singularity at $\vec{q} = \vec{Q}$ i.e., $\chi(q,\omega)|_{\vec{q}=\vec{Q},\omega=0} = \langle\langle S^+(q,t)\ ;\ S^-(-q,t)\rangle\rangle_\omega |_{q=Q,\omega=0} \rightarrow \infty$ where $S^\pm$ are the raising and lowering operators and $\vec{Q}$ is known as the nesting wave vector which determines the periodicity of the SDW. This singularity in the magnetic susecptibility is an artifact of the nesting property of the FS given by

$$\epsilon_{\vec{k}} = -\epsilon_{\vec{k}+\vec{Q}} \tag{1}$$

Now, electron correlations in narrow band systems is best described by the Hubbard model [8]. The interaction term in the Hubbard Hamiltonian can be treated in the mean field approximation to get the SDW state as follows :

$$\begin{aligned} H_I = U\sum_i n_{i\uparrow}n_{i\downarrow} &= \sum_i C^\dagger_{i\uparrow}C_{i\uparrow}C^\dagger_{i\downarrow}C_{i\downarrow} \approx U\sum_i[<C^\dagger_{i\uparrow}C_{i\uparrow}>C^\dagger_{i\downarrow}C_{i\downarrow} + C^\dagger_{i\uparrow}C_{i\uparrow}<C^\dagger_{i\downarrow}C_{i\downarrow}> \\ &- <C^\dagger_{i\downarrow}C_{i\uparrow}>C^\dagger_{i\uparrow}C_{i\downarrow} - <C^\dagger_{i\uparrow}C_{i\downarrow}>C^\dagger_{i\downarrow}C_{i\uparrow}] = \sum_i[Un_i(C^\dagger_{i\uparrow}C_{i\uparrow} + C^\dagger_{i\downarrow}C_{i\downarrow}) \\ &+\Delta^z_i(C^\dagger_{i\uparrow}C_{i\uparrow} - C^\dagger_{i\downarrow}C_{i\downarrow}) + \Delta^+_i C^\dagger_{i\downarrow}C_{i\uparrow} + \Delta^-_i C^\dagger_{i\uparrow}C_{i\downarrow}] \end{aligned} \tag{2}$$

where $n_i = \frac{1}{2}(<C^\dagger_{i\uparrow}C_{i\uparrow}> + <C^\dagger_{i\downarrow}C_{i\downarrow}>)$, $\Delta^z_i = -\frac{U}{2}(<C^\dagger_{i\uparrow}C_{i\uparrow}> - <C^\dagger_{i\downarrow}C_{i\downarrow}>) = -U<S_z>$, $\Delta^+_i = -U<C^\dagger_{i\uparrow}C_{i\downarrow}> = -U<S^-_i>$ and $\Delta^-_i = -U<C^\dagger_{i\downarrow}C_{i\uparrow}> = -U<S^-_i>$

Therefore, the meanfield Hubbard Hamiltonian can be written as,

$$H = -\sum_{ij\sigma} t_{ij}C^\dagger_{i\sigma}C_{j\sigma} + U\sum_i n_i\hat{n}_i + \sum_i \sigma_i.B_i \tag{3}$$

where $\hat{n}_i = C^\dagger_{i\uparrow}C_{i\uparrow} + C^\dagger_{i\downarrow}C_{i\downarrow}$ and $B^z_i = \Delta^z_i = -U<S^z_i> \equiv$ the order parameter for longitudinal magnetization, $B^\pm_i = \Delta^\pm_i = -U<S^\pm_i> \equiv$ transverse magnetization and $\bar{\sigma}_i = \begin{pmatrix} C^\dagger_{i\uparrow} & C^\dagger_{i\downarrow}\end{pmatrix}\bar{\tau}\begin{pmatrix} C_{i\uparrow} \\ C_{i\downarrow}\end{pmatrix}$, where $\bar{\tau} \equiv$ Pauli matrices. The 2^{nd} term of equation (3) corresponds to total charge of the system whereas the 3^{rd} term is the total spin. Hence, eqn. (3) demonstrates that the charge and spin degree of freedom of the Hubbard model is seperated. Now, the SDW state can be described equivalently in terms of either the longitudinal or transverse spin polarization. For example the SDW state with wave vector $\vec{Q}$, having longitudinal spin polarization is

$$< S_i^z > = S_o^z \times \begin{cases} Cos(\vec{Q} \cdot \vec{R}_i) \; for \;\; Spin \; densities \; on \; sites. \\ Sin(\vec{Q} \cdot \vec{R}_i) \; for \;\; Spin \; densities \; on \; bonds. \end{cases} \tag{4}$$

In momentum representation the mean field Hamiltonian for a transverse SDW state becomes

$$H_{SDW} = \sum_{k,\sigma} \epsilon_k C^\dagger_{k,\sigma} C_{k,\sigma} + \Delta_{SDW} \sum_k (C^\dagger_{k+Q\uparrow} C_{k\downarrow} + h.c) \tag{5}$$

where $\Delta_{SDW} = -U \sum_k < C^\dagger_{k\uparrow} C_{k-Q\downarrow} >$, the order parameter for the transverse SDW state. The quasi particle energy spectrum of the SDW state can be writen as $E_k = \sqrt{\epsilon_k^2 + \Delta^2_{SDW}}$ with a gap of $2\Delta_{SDW}$ at the Fermi level. To note, there is a formal similarity of the SDW mean field theory with that of the BCS, in energy spectrum, gap equation, as well as in the collective modes (it is $2\Delta_{SDW}$ in case of the SDW state) [9].

Usually, magnetism and superconductivity are expected to be mutually exclusive phenomena i.e, they are unlikely to occur simultaneously in the same compound. Superconductivity (including in the high temperature superconductors) is known to be due Cooper pair formation of electrons of opposite *spins* and momenta whereas magnetism requires *spin* polarisation. Therefore, naturally one order would inhibit the other. Furthermore, like superconductivity (electron-electron pairing), the SDW is also a result of pair condensation of electron-hole of opposite spins but with a momentum difference of $\vec{Q}$ between the conjugates. Hence, when any of the orders (either the SC or the SDW) set in, the FS is instable with respect to the condensate state. In other words, if one of the phases (say) SDW sets in first, and exists all over the FS, then there will be no carrier available to form cooper pairs and hence no superconductivity. However, in reality we do see the coexistence of the two phases as is already discussed earlier.

The gap due to the SDW state exists all over the FS in case of an isotropic SDW gap transforming the system from metal to insulator. On doping the system with hole, the hole will essentially be produced at the top of lower filled (valence) SDW band. Doping holes or equivalently removal of electrons, locally moves the FS away from perfect nesting resulting in a local suppression of the SDW gap. This is because, the gain in energy to the system in coming down to the SDW state from the normal is being partially violated while taking electrons away. Now, this local suppression of the SDW gap acts as a potential well for the injected hole. On creating two holes it is energetically favourable for them to dig a deeper well and stay together provided the two holes have opposite spins to avoid Pauli exclusion principle. This is however nothing but like a Cooper pair and if such a bag with two holes of opposite spins move coherently the system will be superconducting. This is the essence of Schrieffer's spin bag model for high temperature superconductivity [10] and hence is an example where superconductivity can arise over the SDW state.

The above case is however, physically resonable only when the hole concentration is very small. But in reality superconductivity in most of the systems (specially high T_c systems) appears only after large doping. So, it is likely that the SDW state will be completely suppressed in particular directions of the FS whereras it would still exist in rest part of the FS where it still nests (anisotropic SDW). Such situation may also appear due to particular topology of the FS of a system without doping i.e, the system may have nested pieces of FS only in certain direction and no nesting in other direction resulting in anisotropic SDW state. Now, in the former case where the SDW gap vanishes (i.e, the lower and upper SDW bands mixes together) in certain directions due to loss of FS nesting, the pairing interaction between the SDW quasi particles can take place leading to superconductivity. For a microscopic point of view, the effective attractive interaction between the SDW quasi particle in this picture can be rationalised (Ghosh et al, [10]) as arising due to the exchange of the collective modes of the SDW state. In both these two cases discussed above the origin of superconductivity is fundamentally different from that in conventional superconductors.

In contrast, in the cases where nesting is not perfect due to peculiar topology of the FS, the SDW can occur only in the nested part of the FS wheras superconductivity in the rest part of the FS. But the origin of superconductivity could be due to any other reason including the BCS phonon mechanism. We discuss here this possibility.

The Hamiltonian for the coexistence phase of superconductivity and the SDW state can be obtained as,

$$H = \sum_{k,\sigma} \epsilon_k C^{\dagger}_{k,\sigma} C_{k,\sigma} + \Delta_{SDW} \sum_k (C^{\dagger}_{k+Q\uparrow} C_{k\downarrow} + h.c.) + \Delta \sum_k (C^{\dagger}_{k\uparrow} C^{\dagger}_{-k\downarrow} + h.c.) \tag{6}$$

where $\Delta = -V \sum_k < C^{\dagger}_{k\uparrow} C_{-k\downarrow} >$ with V being the strength of the attractive pairing interaction mediated by some boson exchange. A detailed mean field theory of such coexistence phase [9] are well described in literature. Here we put down the gap equations for the respective gaps in the system as follows.

$$\Delta_{SDW} = (-\frac{U}{4}) \sum_{k,i=1,2} (-1)^i \frac{\Delta_i}{E_i(k)} \tanh \frac{\beta E_i(k)}{2} \tag{7}$$

and

$$\Delta = (\frac{V}{4}) \sum_{k,i=1,2} \frac{\Delta_i}{E_i(k)} \tanh \frac{\beta E_i(k)}{2} \tag{8}$$

with $\Delta_i = (\Delta - (-1)^i \Delta_{SDW})$ and $E_i(k) = \sqrt{\epsilon_k^2 + \Delta_i^2}$.

To note that the equations (7-8) are coupled integral equations in the sense that $\Delta \equiv \Delta(\Delta, \Delta_{SDW})$ and so is $\Delta_{SDW} \equiv \Delta_{SDW}(\Delta, \Delta_{SDW})$. We solve these two gap equations self-consistently numerically. Before we present our numerical results we would like to point out that from equations (7-8) it appears as if there exists two different kinds of modes $\Delta_{1,2} = \Delta \pm \Delta_{SDW}$ indicating that the order parameters can interfere with each other either destructively or constructively. In striking contrast, such situation was not found in the coexistence phase of the charge density wave (CDW) and superconductivity [11] and the quasi particle energy spectrum is given by $E_k = \sqrt{\epsilon_k^2 + W^2 + \Delta^2}$ where W is the CDW gap parameter. Such contrast in behaviour between the SDW and CDW-SC can be rationalized as arising due to the effect of interference between the order parameters of the SDW and SC state which involve the up and down spin electron-hole and electron-electron pairing respectively. Therefore, the electrons with the same spins are likely to compete for both the processes, thereby giving rise to interference.

In solving equations (7-8) we change the momentum sum to integrations with typically 2-D square density of states (DOS). However, while doing so we divide the k-sum into parts such that only in some part of the FS the nesting exists and hence the SDW gap whereas in other parts there is no SDW gap. In other words, the momentum sum is broken up as, $\sum_k = \sum_{k\epsilon\Delta_{SDW}\neq 0} + \sum_{k\epsilon\Delta_{SDW}=0}$ such that the DOS can also be divided into as, $N(0) = N_1(0) + N_2(0)$. $N_1(0)$ denotes the DOS of the region where nesting exists whereas the $N_2(0)$ for the rest of the part of the FS such that $n_1(= \frac{N_1(0)}{N(0)}) + n_2(= \frac{N_2(0)}{N(0)}) = 1$. We emphasis that such division of the DOS is essential in order to solve the two gap equations simultaneously. Now, if one varies n_1 (or $n_2 = 1 - n_1$) which amounts to changing the total SDW gapped region will essentially mimick like doping the system. This is because, if n_1 is large and close to unity it would indicate that the whole FS is gapped by SDW (as happens in half-filled case) and while reducing it will mean to shrink the region of the FS gapped with SDW. For a given set of dimensionless parameters, $\lambda_u(\equiv$ N(0)U)=0.7, $\lambda_v(\equiv$ N(0)V) = 0.702, n_1 =0.6 and the cut-off frequencies for the SDW & SC states Ω_{SDW} = 0.07 eV & Ω_{sc} =0.03 eV, we present below our result of numerical calculation in Fig.1.

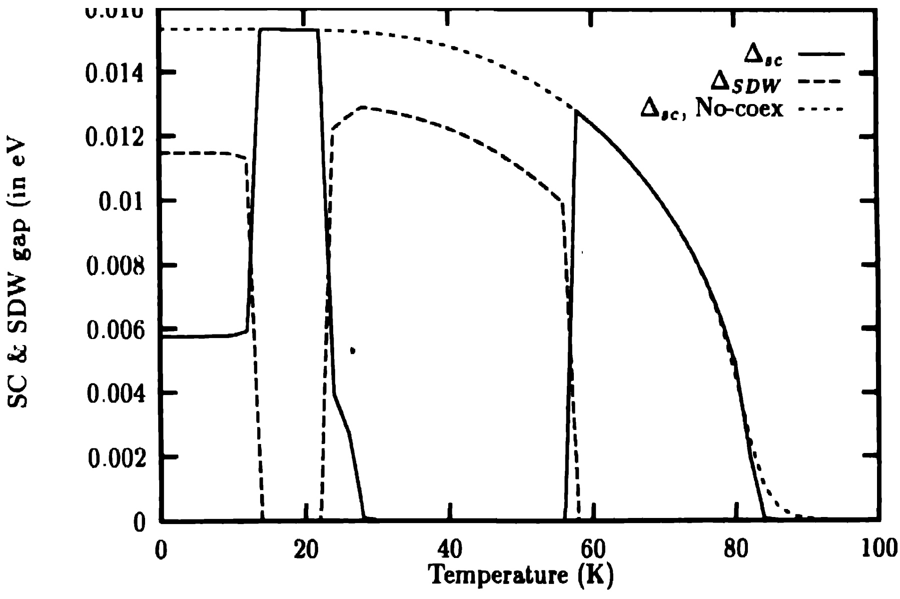

Fig. 1. Thermal variation of the order parameters. The coexistence and reentrance of different phases are worth noticing. The curve with smaller dashes correspond to Δ_{sc} for λ_u = 0.6, show no coexistence with the SDW phase.

For the given set of input parameters mentioned above the superconducting gap opens up (represented by the soild curve) first around 85 K (T_c) inhibiting the SDW gap, then it drops to zero at 56 K where the SDW order sets in and continues up to 23 K. Around the thermal region 23 K – 15 K, the Δ_{SDW} vanishes whereas the Δ_{sc} attains its maximum value. It is only below 15 K where both the SC as well as the SDW order coexist. Clearly, Fig. 1 demonstrates the strong competition between the two orders emphasising the reentrance and coexistence of superconductivity with the SDW state. To our knowledge no such theoretical demonstration exists. This feature is an out come of the typical destructive as well as constructive interference between the SDW and SC ordered parameters described earlier. In order to facilitate that such strong competition between the magnetic order and superconductivity can only happen when the strength of interaction for both the processes are very close, we presented the thermal variation of $\Delta_{sc}(T)$ for $\lambda_u = 0.60$ (short dashed curve). The SDW gap does not appear in this case. Evidently, it indicates the suppression of $\Delta_{sc}(0)$ in presence of the Δ_{SDW} and vice versa. Therefore, the BCS characteristic ratio $\frac{2\Delta}{k_B T_c}$ will not remain constant when both the orders are present. Furthermore, a static magnetic susceptibility calculation within this model will show up in a double reentrant behaviour with respect to temperature, which is in agreement with the experimental observations for Ho-borocarbide systems [12]. Different physical properties in this model, with a complete phase diagram will be published elsewhere. Finally, at this moment it is really hard to predict whether the magnetism in borocarbides (certainly antiferro like) is driven by the SDW formation, as no realistic band structure result exists. In contrast, the reentrance and coexistence of magnetism with superconductivity within our model is consistent with that seen in borocarbides as well as in other systems.

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